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A phase field modelling for multi-scale deformation mechanics of polycrystalline metals

Takuya Uehara ^{a*}^a*Yamagata University, 4-3-16, Jonan, Yonezawa 992-8510, Japan*

Abstract

A phase field modelling to clarify the multi-scale deformation mechanism of polycrystalline metals was undertaken. Modified coupling equations between the phase and stress/strain using a multiphase field model were introduced, and solved numerically under typical test-case conditions. The grain growth process was simulated first, and the microscopic stress distribution was calculated. The microstructural morphology was drastically affected by the stress dependency. The relationship between macroscopic loading and microstructure was then verified by a tensile test. Microstructural rearrangement was induced by macroscopic deformation, and we conclude that the present model is effective for further investigation into the multi-scale deformation mechanics.

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1. Introduction

The mechanical behavior of materials is strongly affected by their microstructure, and hence comprehensive modeling of the microstructure is necessary for a precise estimation of the macroscopic stress and the deformation behavior. A phase field model is a suitable tool for a consideration of the effect of microstructure on the mechanics, since various kinds of microstructure have been generated using the model [1-3]. The fundamental equations have been derived thermodynamically [2], and various kinds of material systems have been studied by adopting a suitable free energy description. For polycrystalline materials, grain growth and re-crystallization simulations have been undertaken using the multiphase field model [4-6]. This model was initially used to describe material systems consisting of multiple phases

* Corresponding author. Tel.: +81-238-26-3285; fax: +81-238-26-3285.

E-mail address: uehara@yz.yamagata-u.ac.jp.

[7,8], and was later extended to polycrystalline materials by treating each crystal grain as an individual phase. Using this model, the grain coarsening process can be simulated while the stable or quasi-equilibrium states of the polycrystalline structure, as observed in ordinal microscopy, is not completely achieved. An understanding of the interaction between the thermal, chemical or metallurgical state and the mechanical behavior has also been developed. Uehara et al. derived the coupling equations that link the phase field and the stress/strain, and demonstrated the generation of microscopic stress distributions in several microstructures [9-11]. However, the evolution of grain morphology was not included in these studies, since it was based on a single phase field model. Therefore, coupling the mechanical field with the multiphase field model is expected to enable more realistic simulations leading to the construction of a framework of multi-scale deformation mechanics.

In this study, we propose a coupling equation for the microstructure formation and the stress distribution, and test case simulations are demonstrated. Following the outline of the equations and the modeled conditions in Sec. 2 and 3, respectively, the simulation results are shown in Sec. 4. First, the grain growth and stress distribution in a polycrystalline structure is simulated. We then give a specific situation where the internal stress affects the microstructure evolution. Finally, a tensile test condition is simulated to show that the interaction between the external macroscopic load and the internal microstructure evolution can be represented by the model, and our conclusions are given in Sec. 5.

2. Fundamental equations

In the original multiphase field model, the phase of the material is defined by N variables ϕ_i , where $i = 1, 2, \dots, N$, and N is the total number of phases that exist in the system. For instance, if the material is on the k -th phase, $\phi_k = 1$, and $\phi_i = 0$ for $i \neq k$, retaining $\sum \phi_i = 1$ is always satisfied. For a polycrystalline model, multiphase field variables are adopted for every grain. The fundamental equations used in this study are summarized below.

$$\dot{\phi}_i = -\frac{2}{n} \sum_{j \neq i} m_{ij} (g_{ij}^c + g_{ij}^p + g_{ij}^g + g_{ij}^m), \quad (1)$$

where,

$$g_{ij}^c = f_{ij} \sqrt{\phi_i \phi_j}, \quad g_{ij}^p = \sum_k (w_{ik} - w_{jk}) \phi_k, \quad g_{ij}^g = \sum_k \frac{1}{2} (a_{ik}^2 - a_{jk}^2) \nabla^2 \phi_k, \quad g_{ij}^m = B_{ij} \sigma^m \phi_i \phi_j. \quad (2)$$

Here, the first to the third terms, g_{ij}^c , g_{ij}^p and g_{ij}^g on the right-hand side of Eq.(1) and their formulae in Eq.(2) are based on the original multiphase field model [8], although the expression is simplified, as well as m_{ij} , f_{ij} , w_{ij} , and a_{ij} , the inter-phase parameters between the i -th and j -th phases, and n , the number of non-zero ϕ_i . The fourth term in Eq.(1) is added in this study to take into account the dependency of the phase change on stress, where σ^m is the mean stress and B_{ij} are inter-phase parameters. This form is introduced as a simple form originating from the elastic strain energy, and a detailed derivation will be reported elsewhere.

For the mechanical field, the stress is calculated using the stress equilibrium equation, $\partial \sigma_{pq} / \partial x_q = 0$ ($p, q = 1, 2$) in two dimensional space. As a constitutive relation, isotropic elasticity is assumed. Every grain is assumed to have a different mass density and elastic properties such as Young's modulus E and Poisson's ratio ν . The difference in the mass density corresponds to the phase transformation dilatation coefficient β from the original phase to the new phase. These values are differently given for every grain, and are denoted β_i , E_i and ν_i , while only β_i is varied in this study to generate simple stress states to enable us to concentrate on the representation of the model's efficiency.

3. Simulation model and conditions

The fundamental equations described in the previous section are verified by considering two situations. One is grain growth from an original phase (denoted by ϕ_0) to a precipitated phase, where the grains in the new phase are distinguished using the multiphase field (denoted by ϕ_1 - ϕ_N). To determine the efficiency of the stress-dependent effects on grain growth, a density variation is assigned to every grain to generate stress distribution in the material. The second situation is tensile loading, where the microstructure evolution induced by macroscopic deformation is evaluated.

The phase field equation (1) is solved using the finite difference method (FDM), while the stress field is calculated by the finite element method (FEM). The lattice points for FDM and the nodes for FEM are linked. The parameters m_{ij} , a_{ij} and w_{ij} are constant at m_0 , a_0 and w_0 , respectively for every inter-phase relation (i.e. for $i \neq j$), and 0 for $i = j$. Another parameter f_{ij} is constant for the phase transformation from the original phase to the new phase, and is neglected for the inter-grain interaction; i.e. $f_{ij} = f_0$ for $i=0$, $f_{ij} = -f_0$ for $j=0$, and $f_{ij} = 0$ for all other cases. The values used for the parameters are as follows: $m_0=1.0$, $f_0=10.0$, $a_0=2.5$, $w_0=0.5$, the grid interval $\Delta x (= \Delta y)=1.0$, the number of grids $N_x (=N_y)=120$, and the time increment $\Delta t=0.032$. The volumetric parameter β_i is varied for every grain between β_0 and β_1 , while Young's modulus and Poisson's ratio are identical for every grain at $E = 120$ and $\nu = 0.3$. All the boundaries are mechanically fixed, while periodic boundary conditions are applied for the phase field. Note that all these parameters are non-dimensionalized.

4. Results and discussion

4.1. Grain growth

The grain growth process is simulated to confirm the characteristic behavior of the multiphase field model. A regular arrangement of 16 grain nuclei is set in a uniform original phase, and the grain growth processes for the different grain numbering are shown. The grain number is assigned randomly, and the results for the following two cases are discussed. Case 1; every grain is surrounded by different types of grains as shown in Fig. 1(a). Case 2; some of the neighboring grains have the same numbers as shown in Fig. 1(b). In Case 1, every grain forms a hexagonal shape, and the microstructure is stable since triple junctions with 120° angles are stable in this model. In Case 2, on the contrary, some connected grains appear, and differently-shaped grains form. For instance, the connected grain indicated by the white arrow in Fig. 1(b)(ii) is initially formed. This grain grows larger, and the neighboring small grains tend to shrink. This leads to the whole microstructure becoming unstable, and grain rearrangement is initiated. Once this happens, the change in shape continues until all the grains are connected to form a single crystal.

Figure 2 shows the evolution of grain shape (left) and stress distribution (right). The color in the left-hand figures is depicted by $\Sigma \phi_i^2 (1 - \phi_i)^2$, in which the demarcated regions correspond to grain boundaries. The right-hand figures represent the mean stress $\sigma_x + \sigma_y$. The volumetric parameter β_i is varied between

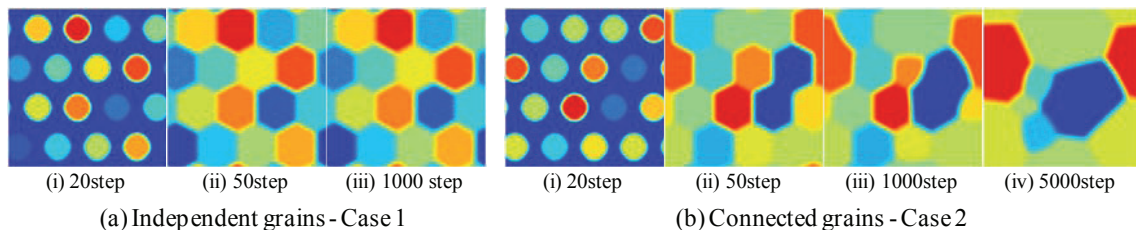


Fig. 1. Phase transformation and grain growth shown with the grain numbers.

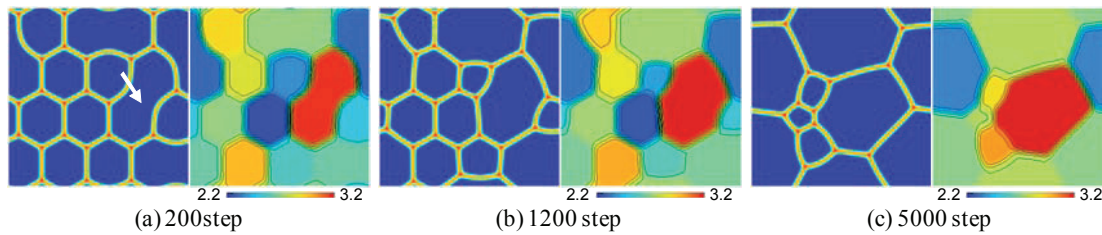


Fig. 2. Grain growth without stress-dependency: grain boundaries (left) and mean stress (right).

$\beta_0 = -0.015$ and $\beta_1 = -0.005$, where a negative value indicates shrinkage upon transformation from the original phase. The stress-dependent term g^m in Eq.(1) is neglected here. Because of the fixed boundary condition, tensile stress is generated, and the values are different for every grain. As a matter of course, the stress distribution changes as grain coarsening continues. Since the influence of stress on the phase field is not considered in this section, the grain growth is independent of the stress values of the grains. This is to be compared with the results in the next section.

4.2. Stress-dependent microstructure formation

Grain growth in the previous section was determined by the nature of the multiphase field model, and is caused by the energy barrier at the grain boundaries. In this section, the stress-induced term g^m is introduced with $B_{ij} = 1.0$ for every i and j . A simulation under the same conditions as in Case 2 is demonstrated. In the case that was shown in Fig. 2, incidentally enlarged grains grow larger only due to the balance of grain boundary energy. Figure 3 shows the results obtained when the stress-dependent term is included. The initially large grain, indicated with a white arrow, has a relatively large tensile stress. This grain shrinks as time progresses, and diminishes before the 200th time step. At the same time, the neighboring grains, which have relatively small tensile stress, grow larger, and a completely different microstructure is obtained. From the viewpoint of elastic strain energy, it is advantageous for this grain to shrink to reduce the total energy of the system. Grain shrinkage occurs in this case because the strain-energy effect is larger than the grain boundary effect.

Figure 4 shows the stress evolution during grain growth without and with the stress dependency, which corresponds to the processes shown in Figs. 2 and 3, respectively. When the stress dependency is

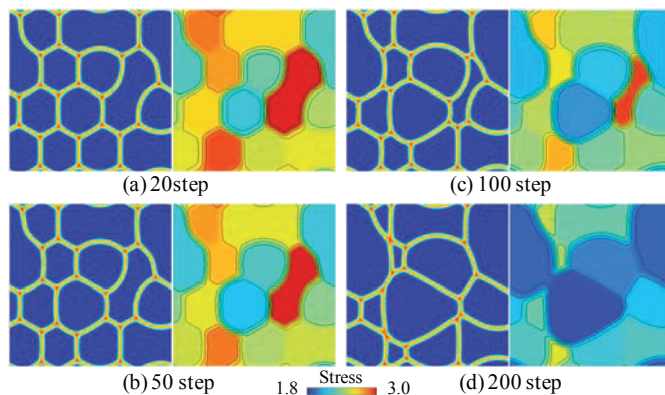


Fig. 3. Grain growth with stress-dependency: grain boundaries (left) and mean stress (right).

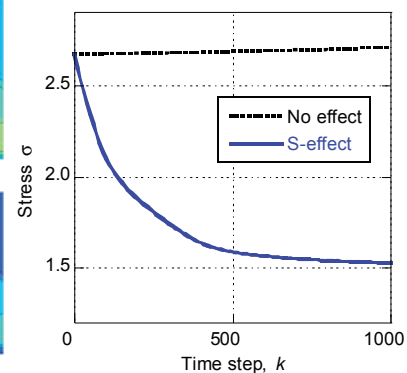


Fig. 4. Stress evolution during grain growth.

considered, the stress is reduced as the grain grows, as shown by the blue solid line, while it increases slightly when the dependency is neglected. This shows that the stress-induced term effectively accounts for the strain energy reduction.

4.3. Tensile-test simulation

Tensile-test conditions are simulated in this section to verify that the influence of macroscopic loading on the microstructure is effectively described by this model. A tensile load is imposed in the y direction by giving a constant increment Δl_y to the y edge every 200 time steps. To show the stress effect clearly, a larger variance in the volumetric parameter $\beta_0 = -0.015$ and $\beta_1 = +0.015$ is applied.

Figure 5 shows the microstructure evolution and the mean stress distribution under tensile loading, and the corresponding stress evolution is shown in Fig. 6. When the model is extended in the y direction, every hexagonal grain is homogeneously extended. When the stress dependency is neglected, nothing happens and the extended hexagonal shapes are retained, as shown in Fig. 6(a). When the stress dependency is included, the microstructure drastically changes its morphology, as shown in Fig. 5. In the early stage, the grains that have a relatively large tensile stress start to shrink, and the grains that have compressive stress grow larger so that the total strain energy is reduced. At this stage, the sizes of grains change, but they retain their hexagonal shapes. As the macroscopic tensile strain increases, the three edges of the small grain become shorter, and the grain shape is close to a triangle, as shown in Fig. 5(c). The microstructure

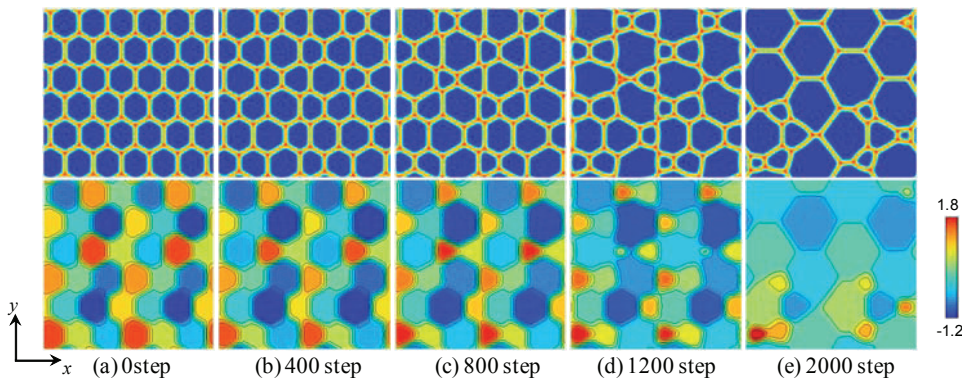


Fig. 5. Microstructure evolution due to external tensile loading: Grain boundaries (top) and mean stress distribution (bottom).

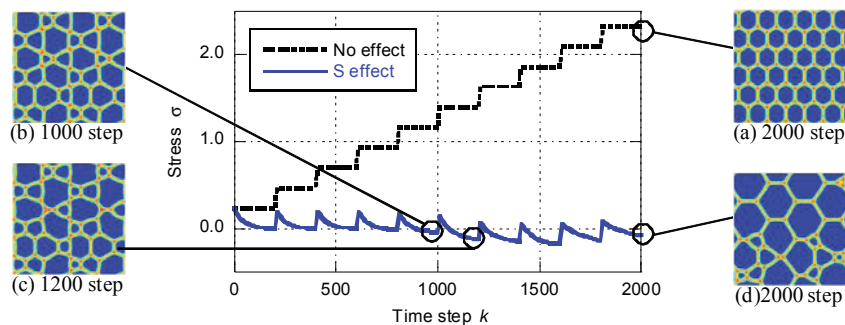


Fig. 6. Stress evolution during tensile test when a microstructure rearrangement occurs by considering the stress dependency (blue solid line), and when no change occurs (black dashed line).

then becomes unstable, and the morphology changes drastically, as shown in Fig. 5(d). Once unstable growth is initiated, the grain growth continues not only by the strain-energy effect but also by the grain boundary effect. As shown in Fig. 6, when no change occurs in the microstructure, the stress increases constantly to the imposed strain as an elastic behavior. On the contrary, when microstructure rearrangement occurs, the macroscopic stress is released gradually after an instantaneous increase due to the external load. This stress release is apparently caused by microstructural rearrangement. The same behavior is observed for every load before the 1000th time step, where the stress approaches 0. The convergent value shifts slightly after the 1000th step. This is because the change in microstructure is driven by the strain-effect and also by the grain boundary effect, which is independent of the stress term. This is shown in the morphologically unstable state after the 1000th step, as shown in Figs. 5 (d) and (e).

5. Conclusion

A phase field model that represents the coupling effects between a microstructure and the stress distribution was proposed, and the following simulations were carried out. The microscopic stress distribution during the grain growth was calculated, and it was shown that the morphology of the microstructure varies drastically by considering the stress dependency of the multiphase field evolution. In a tensile-test simulation, a microstructure rearrangement was induced by the external macroscopic load. These results, therefore, are promising for the applicability of the presented model to further investigations into multi-scale deformation mechanics. As future work, the crystal orientation of every grain is to be considered, since the orientation affects both the grain boundary energy and the mechanical properties of every grain. For a more precise estimation of the stress distribution, the anisotropy in the elasticity is to be taken into account.

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